10/540,993

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                  Zentralblatt
 NEWS 3 OCT 19 BEILSTEIN updated with new compounds
 NEWS 4 NOV 15 Derwent Indian patent publication number format enhanced
 NEWS 5 NOV 19 WPIX enhanced with XML display format
 NEWS 6 NOV 30 ICSD reloaded with enhancements
 NEWS 7 DEC 04 LINPADOCDB now available on STN
 NEWS 8 DEC 14 BEILSTEIN pricing structure to change
 NEWS 9 DEC 17 USPATOLD added to additional database clusters
 NEWS 10 DEC 17 IMSDRUGCONF removed from database clusters and STN
 NEWS 11 DEC 17 DGENE now includes more than 10 million sequences
 NEWS 12 DEC 17 TOXCENTER enhanced with 2008 MeSH vocabulary in
                  MEDLINE segment
 NEWS 13 DEC 17 MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
 NEWS 14 DEC 17 CA/CAplus enhanced with new custom IPC display formats
 NEWS 15 DEC 17 STN Viewer enhanced with full-text patent content
                  from USPATOLD
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 NEWS 17 JAN 16 CAS patent coverage enhanced to include exemplified
                  prophetic substances
 NEWS 18 JAN 28 USPATFULL, USPAT2, and USPATOLD enhanced with new
                  custom IPC display formats
 NEWS 19 JAN 28 MARPAT searching enhanced
 NEWS 20 JAN 28 USGENE now provides USPTO sequence data within 3 days
                  of publication
 NEWS 21 JAN 28 TOXCENTER enhanced with reloaded MEDLINE segment
 NEWS 22 JAN 28 MEDLINE and LMEDLINE reloaded with enhancements
 NEWS 23 FEB 08 STN Express, Version 8.3, now available
 NEWS 24 FEB 20 PCI now available as a replacement to DPCI
 NEWS 25 FEB 25 IFIREF reloaded with enhancements
 NEWS 26 FEB 25 IMSPRODUCT reloaded with enhancements
 NEWS 27 FEB 29 WPINDEX/WPIDS/WPIX enhanced with ECLA and current
                  U.S. National Patent Classification

 NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
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McIntosh

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STRUCTURE FILE UPDATES:   14 MAR 2008  HIGHEST RN 1008127-41-0
DICTIONARY FILE UPDATES:  14 MAR 2008  HIGHEST RN 1008127-41-0

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=> e 6-(2-fluorobenzylamino)purine riboside/cn
E1            1     6-(2-FLUOROBENZYL)-N-(3-METHOXYPROPYL)-5,7-DIMETHYLPYRAZOLO(
                    1,5-A)PYRIMIDINE-3-CARBOXAMIDE/CN
E2            1     6-(2-FLUOROBENZYLAMINO)PURINE/CN
E3            0 --> 6-(2-FLUOROBENZYLAMINO)PURINE RIBOSIDE/CN
E4            1     6-(2-FLUOROBIPHENYL-4-YL)-3-((1-ISOPROPYLPIPERIDIN-3-YL)METH
                    YL)-2-(2-METHYLPHENYL)QUINAZOLIN-4(3H)-ONE MONOTRIFLUOROACET
                    ATE/CN
E5            1     6-(2-FLUOROETHOXY)-2-(2-(2-(MORPHOLIN-4-YL)THIAZOL-5-YL)VINY
                    L)BENZOXAZOLE/CN
E6            1     6-(2-FLUOROETHOXY)-2-METHYL-3-(4-(3-(PIPERIDIN-1-YL)PROPOXY)
                    PHENYL)-4(3H)-QUINAZOLINONE/CN
E7            1     6-(2-FLUOROETHOXY)-2-METHYL-3-(4-(3-(PYRROLIDIN-1-YL)PROPOXY
                    )PHENYL)-4(3H)-QUINAZOLINONE/CN
E8            1     6-(2-FLUOROETHYL)-2-(3-FLUOROPYRIDIN-4-YL)-5,6-DIHYDRO-1H-PY
                    RROLO(3,4-B)PYRROL-4-ONE/CN
E9            1     6-(2-FLUOROETHYL)-2-(PYRIDIN-4-YL)-5,6-DIHYDRO-1H-PYRROLO(3,
                    4-B)PYRROL-4-ONE/CN
E10           1     6-(2-FLUOROMETHYL-2-ACETOXYPROPYL)-2,4-DIHYDROXY-5-METHYLPYR
                    IMIDINE/CN
E11           1     6-(2-FLUOROMETHYL-2-ACETOXYPROPYL)-2,4-DIMETHOXY-5-METHYLPYR
                    IMIDINE/CN
E12           1     6-(2-FLUOROMETHYL-2-HYDROXYPROPYL)-2,4-DIHYDROXY-5-METHYLPYR
                    IMIDINE/CN

=> s e2
L1            1 "6-(2-FLUOROBENZYLAMINO)PURINE"/CN

=> d l1

L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   67023-50-1  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   9H-Purin-6-amine, N-[(2-fluorophenyl)methyl]-  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   1H-Purin-6-amine, N-[(2-fluorophenyl)methyl]- (9CI)
OTHER NAMES:
CN   6-(2-Fluorobenzylamino)purine
CN   N-[(2-Fluorophenyl)methyl]-1H-purin-6-amine
MF   C12 H10 F N5
LC   STN Files:   CA, CAPLUS, CASREACT, TOXCENTER, USPAT2, USPATFULL
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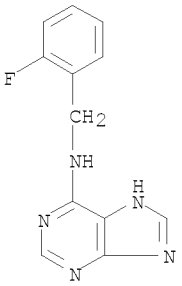

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)
7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       8.07       8.28

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FILE COVERS 1907 - 16 Mar 2008  VOL 148 ISS 12
FILE LAST UPDATED: 14 Mar 2008  (20080314/ED)

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=> s l1
L2            7 L1

=> s l2 and riboside
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            840 RIBOSIDES
           4771 RIBOSIDE
                  (RIBOSIDE OR RIBOSIDES)
L3            0 L2 AND RIBOSIDE

=> s l2 and ribose
          29374 RIBOSE
            176 RIBOSES
          29445 RIBOSE
                  (RIBOSE OR RIBOSES)
L4            0 L2 AND RIBOSE

=> d bib abs hitstr 1-7 l2

L2   ANSWER 1 OF 7  CAPLUS  COPYRIGHT 2008 ACS on STN
AN   2008:68804  CAPLUS
DN   148:127706
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TI Cosmetic and pharmaceutical compositions containing N6-substituted adenines with anticancer and antisenescent and immunosuppresive properties
IN Popa, Igor; Holub, Jan; Lenobel, Rene; Werbrouck, Stefaan; Dolezal, Karel; Strnad, Miroslav; Zatloukal, Marek; Massino, Frank J.
PA Czech Rep.
SO U.S. Pat. Appl. Publ., 43pp., Cont.-in-part of U.S. Ser. No. 485,091.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2008014227	A1	20080117	US 2007-779828	20070718
CZ 294535	B6	20050112	CZ 2001-2818	20010802
WO 2003040144	A2	20030515	WO 2002-CZ45	20020801
WO 2003040144	A3	20040226		
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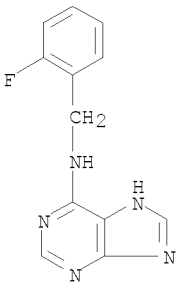
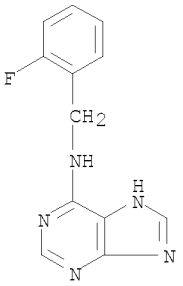
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
NZ 538596	A	20060929	NZ 2002-538596	20020801
NZ 538597	A	20060929	NZ 2002-538597	20020801
US 2005043328	A1	20050224	US 2004-485091	20040907
US 7279482	B2	20071009		
PRAI CZ 2001-2818	A	20010802		
WO 2002-CZ45	W	20020801		
US 2004-485091	A2	20040907		
NZ 2002-531086	A1	20020801		

AB Novel heterocyclic derivs. based on N6-substituted adenine, having anticancer, mitotic, immunosuppressive and antisenescent properties for plant, animal and human cells and methods of their preparation Included are also pharmaceutical compns., cosmetic prepns. and growth regulators, which contain these derivs. as active compound and the use of these derivs. for the preparation of drugs, cosmetic prepns., in biotechnol. processes, in cosmetics and in agriculture.
IT 67023-50-1P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); COS (Cosmetic use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(cosmetic and pharmaceutical compns. containing N6-substituted adenines with anticancer and antisenescent and immunosuppresive properties)
RN 67023-50-1 CAPLUS
CN 9H-Purin-6-amine, N-[(2-fluorophenyl)methyl]- (CA INDEX NAME)



L2 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:1251923 CAPLUS
DN 148:91486
TI The first platinum(IV) complexes involving aromatic cytokinins or cyclin-dependent kinase inhibitors derived from 6-benzylaminopurine: X-ray structures of (BohH22+)[PtCl6]·H2O and

(RosH22+)2[PtCl6]Cl2·4H2O
AU Travnicek, Zdenek; Popa, Igor; Cajan, Michal; Herchel, Radovan; Marek, Jaromir
CS Department of Inorganic Chemistry, Palacky University, Olomouc, CZ-771 47, Czech Rep.
SO Polyhedron (2007), 26(18), 5271-5282
CODEN: PLYHDE; ISSN: 0277-5387
PB Elsevier B.V.
DT Journal
LA English
AB Pt(IV) complexes with cytokinins or CDK-inhibitors derived from 6-benzylaminopurine (Bap) [PtIV(LH+)Cl5], where LH+ stands for protonated form of the Bap derivative, Boh = 6-(benzylamino)-2-[(3-hydroxypropyl)amino]-9-isopropylpurine, bohemine and Ros = 6-(benzylamino)-2-[(1-hydroxymethylpropyl)amino]-9-isopropylpurine, roscovitine, were prepared They were fully characterized by microanal., conductivity, FTIR, 1H, 13C, 15N and 195Pt NMR and ES+ mass spectroscopy. The cytokinin mol. is coordinated via N9 atom to Pt(IV) and N1, N7-protonated in case of the Boh complexes, and N7 coordinated and N1-protonated in case of bohemine and Ros complexes with CDK inhibitors. Predicted mol. geometries of the complexes were supported by DFT calcns. at the B3LYP level with the 6-311+G**/LANL2DZ and aug-cc-pVDZ/LANL2DZ basis sets. All of the compds. were tested in vitro for their cytotoxicity against four human cancer cell lines: malignant melanoma (G361), osteogenic sarcoma (HOS), chronic myelogenous erythroleukemia (K562) and breast adenocarcinoma (MCF7). The best result was achieved for Ros complex, where IC50 = 17 μM against K562. The mol. structures of two ionic pair compds. (BohH22+)[PtCl6]·H2O and (RosH22+)2[PtCl6]Cl2·4H2O were determined by a single crystal x-ray anal.
IT 67023-50-1, 6-(2-Fluorobenzylamino)purine
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation with platinum)
RN 67023-50-1 CAPLUS
CN 9H-Purin-6-amine, N-[(2-fluorophenyl)methyl]- (CA INDEX NAME)



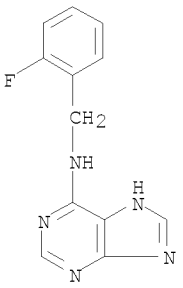
RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:1301890 CAPLUS
DN 144:120922
TI Preparation and biological activity of 6-benzylaminopurine derivatives in plants and human cancer cells
AU Dolezal, Karel; Popa, Igor; Krystof, Vladimir; Spichal, Lukas; Fojtikova, Martina; Holub, Jan; Lenobel, Rene; Schmuelling, Thomas; Strnad, Miroslav
CS Laboratory of Growth Regulators, Palacky University and Institute of Experimental Botany AS CR, Olomouc, 783 71, Czech Rep.
SO Bioorganic & Medicinal Chemistry (2006), 14(3), 875-884
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 144:120922
AB To study the structure-activity relationships of aromatic cytokinins, the cytokinin activity at both the receptor and cellular levels, as well as CDK inhibitory and anticancer properties of 38 6-benzylaminopurine (BAP) derivs. were compared in various in vitro assays. The compds. were prepared

by the condensation of 6-chloropurine with corresponding substituted benzylamines. The majority of synthesized derivs. exhibited high activity in all three of the cytokinin bioassays employed (tobacco callus, wheat senescence and Amaranthus bioassay). The highest activities were obtained in the senescence bioassay. For some compds. tested, significant differences of activity were found in the bioassays used, indicating that diverse recognition systems may operate and suggesting that it may be possible to modulate particular cytokinin-dependent processes with specific compds. Position-specific steric and hydrophobic effects of different Ph ring substituents on the variation of biol. activity were confirmed. In contrast to their high activity in bioassays, the BAP derivs. were recognized with much lower sensitivity than trans-zeatin in both Arabidopsis thaliana AHK3 and AHK4 receptor assays. The compds. were also investigated for their effects on cyclin-dependent kinase 2 (CDK2) and for antiproliferative properties on cancer and normal cell lines. Several of the tested compds. showed stronger inhibitory activity and cytotoxicity than BAP. There was also a significant pos. correlation of the inhibitory effects on human and plant CDKs with cell proliferation of cancer and cytokinin-dependent tobacco cells, resp. This suggests that at least a part of the antiproliferative effect of the new cytokinins was due to the inhibition of CDK activity.

IT 67023-50-1P
RL: AGR (Agricultural use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and biol. activity of 6-benzylaminopurine derivs. in plants and human cancer cells)

RN 67023-50-1 CAPLUS
CN 9H-Purin-6-amine, N-[(2-fluorophenyl)methyl]- (CA INDEX NAME)



RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

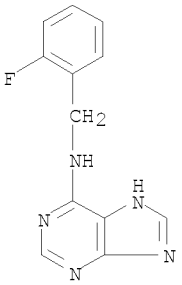
L2 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:1112164 CAPLUS
DN 144:31637
TI Palladium(II) complexes containing cytokinins derived from 6-benzylaminopurine
AU Travnicek, Zdenek; Sipl, Michal; Popa, Igor
CS Department of Inorganic Chemistry, Palacky University, Olomouc, 771 47, Czech Rep.
SO Journal of Coordination Chemistry (2005), 58(16), 1513-1521
CODEN: JCCMBQ; ISSN: 0095-8972
PB Taylor & Francis Ltd.
DT Journal
LA English
OS CASREACT 144:31637
AB Pd(II) complexes [Pd(LH+)Cl3] (1-12) containing 6-benzylaminopurine derivs. were prepared [L = 6-(2-methoxybenzylamino)purine (1), 6-(3-methoxybenzylamino)purine (2), 6-(4-methoxybenzylamino)purine (3), 6-(2-hydroxy-benzylamino)purine (4), 6-(3-hydroxybenzylamino)purine (5), 6-(4-hydroxybenzylamino) purine (6), 6-(2-fluorobenzylamino)purine (7), 6-(3-fluorobenzylamino)purine (8), 6-(4-fluorobenzylamino)purine (9), 6-(2-chlorobenzylamino)purine (10), 6-(3-chlorobenzylamino) purine (11) and 6-(4-chlorobenzylamino)purine (12)]. The compds. were characterized by elemental anal., IR, ES+ MS and 1H- and 13C-NMR spectroscopy, and two of them, 6 and 12, also by TG/DSC analyses. The complexes were screened

in vitro against the four human tumor cell lines G-361, HOS, K-562 and MCF7. No complexes showed significant cytotoxicity, with all IC50 values >100 μM. There is no marked difference in relative cytotoxicity between the complexes and the free ligands.

IT 67023-50-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(coordination to tetrachloropalladate(2-))

RN 67023-50-1 CAPLUS

CN 9H-Purin-6-amine, N-[(2-fluorophenyl)methyl]- (CA INDEX NAME)



RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2003:376865 CAPLUS

DN 138:385444

TI Preparation of substituted adenines as drugs, cosmetics, and agrochemical growth regulators.

IN Dolezal, Karel; Popa, Igor; Holub, Jan; Lenobel, Rene; Werbrouck, Stefaan; Strnad, Miroslav; Zatloukal, Marek

PA Ustav Experimentalni Botaniky Akademie Ved Ceske Republiky, Czech Rep.

SO PCT Int. Appl., 67 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003040144	A2	20030515	WO 2002-CZ45	20020801
WO 2003040144	A3	20040226		
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EP 1419157	A2	20040519	EP 2002-750769	20020801
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SG 119228	A1	20060228	SG 2004-3857	20020801
NZ 538596	A	20060929	NZ 2002-538596	20020801
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SG 127738	A1	20061229	SG 2004-5059	20020801
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OS MARPAT 138:385444

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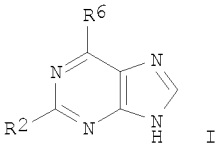


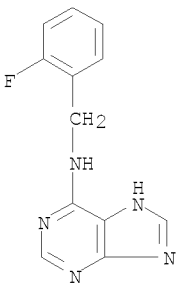
I

AB Title compds. [I; R2 = H, halo, OH, alkoxy, amino, hydrazo, SH, CO2H, cyano, NO2, amido, sulfo, sulfamido, acylamino, acyloxy, cycloalkyl, etc.; R6 = (substituted) alkyl, cycloalkyl, aryl, heterocyclyl, heteroaryl, aralkyl, cycloalkylalkylalkyl, amido, sulfo, etc.], were prepared Thus, 6-chloropurine, 3-chlorobenzylamine, and Et3N were heated in BuOH at 90° for 4 h to give 95% 6-(3-chlorobenzylamino)purine. This showed IC50 = 148.6 μM against G-361 cancer cells.

IT 67023-50-1P, 6-(2-Fluorobenzylamino)purine
RL: AGR (Agricultural use); BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of substituted adenines as drugs, cosmetics, and agrochem. growth regulators)

RN 67023-50-1 CAPLUS

CN 9H-Purin-6-amine, N-[(2-fluorophenyl)methyl]- (CA INDEX NAME)



L2 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1989:540297 CAPLUS

DN 111:140297

TI Research on the constituents of ginger in different preparations

AU Ye, Dingjiang; Ding, Anwei; Guo, Rong

CS Nanjing Coll. Tradit. Chin. Med., Nanjing, Peop. Rep. China

SO Zhongguo Zhongyao Zazhi (1989), 14(5), 278-80
CODEN: ZZZAE3; ISSN: 1001-5302

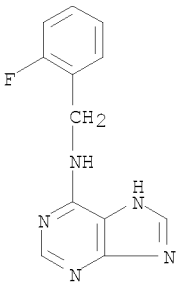
DT Journal

LA Chinese

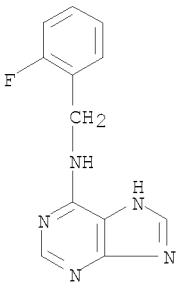
AB The constituents of ginger (Zingiber officinale) prepared by different processes (cold dried, hot dried, or baked at 220°) were compared by column chromatog. and mass spectra.

IT 67023-50-1, N-[(2-Fluorophenyl)methyl]-1H-purin-6-amine
RL: BIOL (Biological study)
(of ginger, processing effect on)

RN 67023-50-1 CAPLUS
CN 9H-Purin-6-amine, N-[(2-fluorophenyl)methyl]- (CA INDEX NAME)



L2 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1978:439623 CAPLUS
DN 89:39623
OREF 89:6115a,6118a
TI In vitro cytokinin binding to a particulate fraction of tobacco cells
AU Sussman, Michael R.; Kende, Hans
CS Plant Res. Lab., Michigan State Univ., East Lansing, MI, USA
SO Planta (1978), 140(3), 251-9
CODEN: PLANAB; ISSN: 0032-0935
DT Journal
LA English
AB At least 2 types of cytokinin-binding sites were present in a particulate fraction of tobacco (Nicotiana tabacum) cells that sediments at 80,000 + g. The major binding component had a low affinity towards cytokinins, was resistant to heating at 100°, and was not specific for biol. active cytokinin analogs. The 2nd site occurred in much lower frequency, was heat labile, showed high affinity towards cytokinins, and was specific for biol. active analogs of the hormone. The low-affinity binding site showed some of the same features as talcum powder, a non-biol. material which binds cytokinins in a nonspecific fashion. The properties of the high-affinity binding site are consistent with the expected characteristics of a cytokinin receptor. However, the role of the observed high-affinity binding site with regard to the biol. action of cytokinins is not yet known.
IT 67023-50-1
RL: BIOL (Biological study)
(binding of, to particulate fraction of tobacco cells)
RN 67023-50-1 CAPLUS
CN 9H-Purin-6-amine, N-[(2-fluorophenyl)methyl]- (CA INDEX NAME)



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FULL ESTIMATED COST

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                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                   -5.60      -5.60

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L5      STRUCTURE UPLOADED

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SAMPLE SCREEN SEARCH COMPLETED -      441 TO ITERATE

100.0% PROCESSED      441 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         7561 TO    10079
PROJECTED ANSWERS:               0 TO        0

L6            0 SEA SSS SAM L5

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FULL SCREEN SEARCH COMPLETED -     8369 TO ITERATE

100.0% PROCESSED     8369 ITERATIONS                              4 ANSWERS
SEARCH TIME: 00.00.01

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                                                      ENTRY    SESSION
FULL ESTIMATED COST                                  181.12     233.23

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)       SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                   0.00      -5.60

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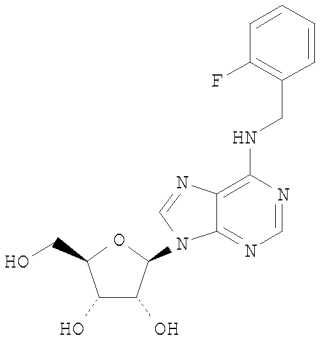
FILE COVERS 1907 - 16 Mar 2008 VOL 148 ISS 12
FILE LAST UPDATED: 14 Mar 2008 (20080314/ED)

=> s l7
L8 15 L7

=> d bib abs hitstr 1-15 l8

L8 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:474159 CAPLUS
DN 147:143613
TI Preparation, biological activity and endogenous occurrence of N6-benzyladenosines
AU Dolezal, Karel; Popa, Igor; Hauserova, Eva; Spichal, Lukas; Chakrabarty, Kuheli; Novak, Ondrej; Krystof, Vladimir; Voller, Jiri; Holub, Jan; Strnad, Miroslav
CS Laboratory of Growth Regulators, Palacky University & Institute of Experimental Botany AS CR, Olomouc, 783 71, Czech Rep.
SO Bioorganic & Medicinal Chemistry (2007), 15(11), 3737-3747
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier Ltd.
DT Journal
LA English
OS CASREACT 147:143613
GI



I

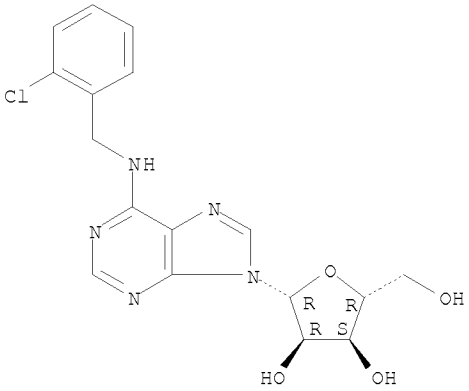
AB Cytokinin activity of forty-eight 6-benzyladenosine derivs., e.g. I, at both the receptor and cellular levels as well as their anticancer properties were compared in various in vitro assays. The compds. were prepared by the condensation of 6-chloropurine riboside with corresponding substituted benzylamines and characterized by standard collection of physico-chemical methods. The majority of synthesized derivs. exhibited high activity in all three of the cytokinin bioassays used (tobacco callus, wheat leaf senescence and Amaranthus bioassay). The highest activities were observed in the senescence bioassay. For several of the compds. tested, significant differences in activity were found between the bioassays used, indicating that diverse recognition systems may operate. This suggests that it may be possible to modulate particular cytokinin-dependent processes with specific compds. In contrast to their high activity in bioassays, the tested compds. were recognized with only very low

sensitivity in both Arabidopsis thaliana AHK3 and AHK4 receptor assays. The prepared derivs. were also investigated for their antiproliferative properties on cancer and normal cell lines. Several of them showed very strong cytotoxic activity against various cancer cell lines. On the other hand, they were not cytotoxic for normal murine fibroblast (NIH/3T3) cell line. This anticancer activity of cytokinin ribosides may be important, given that several of them occur as endogenous compds. in different organisms.

IT 23707-32-6P 101565-87-1P 288087-35-4P
RL: AGR (Agricultural use); PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzyladenosines via condensation of chloropurine riboside with benzylamines, and their cytokinin, antitumor activity and endogenous occurrence)

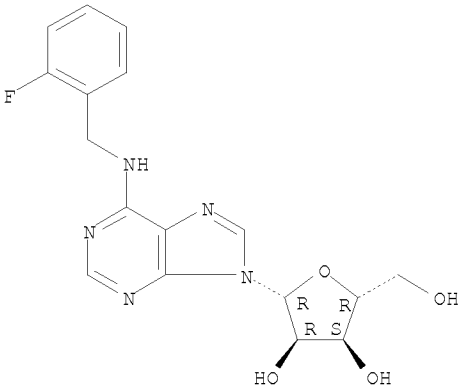
RN 23707-32-6 CAPLUS
CN Adenosine, N-[(2-chlorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



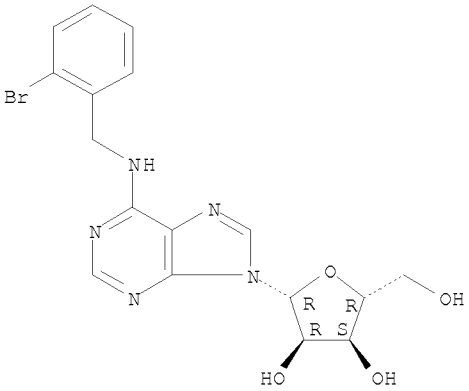
RN 101565-87-1 CAPLUS
CN Adenosine, N-[(2-fluorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



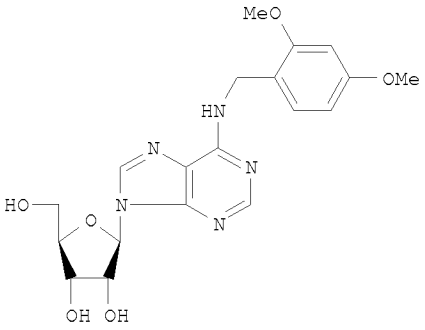
RN 288087-35-4 CAPLUS
CN Adenosine, N-[(2-bromophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:397569 CAPLUS
DN 147:694
TI Synthesis, biological evaluation and molecular modeling studies of N6-benzyladenosine analogues as potential anti-toxoplasma agents
AU Kim, Young Ah; Sharon, Ashoke; Chu, Chung K.; Rais, Reem H.; Al Safarjalani, Omar N.; Naguib, Fardos N. M.; El Kouni, Mahmoud H.
CS University of Georgia College of Pharmacy, Athens, GA, 30602, USA
SO Biochemical Pharmacology (2007), 73(10), 1558-1572
CODEN: BCPCA6; ISSN: 0006-2952
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 147:694
GI



I

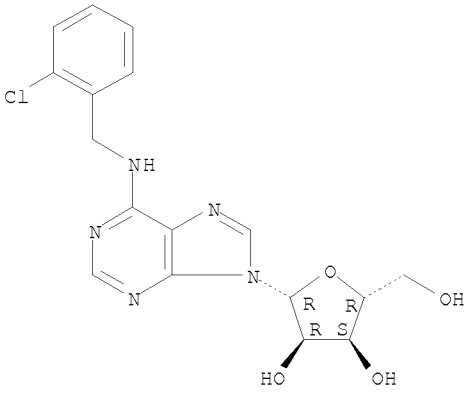
AB Toxoplasma gondii is an opportunistic pathogen responsible for toxoplasmosis. T. gondii is a purine auxotroph incapable of de novo purine biosynthesis and depends on salvage pathways for its purine requirements. Adenosine kinase (EC.2.7.1.20) is the major enzyme in the salvage of purines in these parasites. 6-Benzylthioinosine and analogs were established as "subversive substrates" for the T. gondii, but not for the human adenosine kinase. Therefore, these compds. act as selective antitoxoplasma agents. In the present study, a series of N6-benzyladenosine analogs were synthesized from 6-chloropurine riboside with substituted benzylamines via solution phase parallel synthesis. These N6-benzyladenosine analogs were evaluated for their binding affinity to purified T. gondii adenosine kinase. Furthermore, the antitoxoplasma efficacy and host toxicity of these compds. were tested in cell culture. Certain substituents on the aromatic ring improved binding affinity to T. gondii adenosine kinase when compared to the unsubstituted N6-benzyladenosine. Similarly, varying the type and position of the substituents on the aromatic ring led to different degrees of potency and

selectivity as antitoxoplasma agents. Among the synthesized analogs, N6-(2,4-dimethoxybenzyl)adenosine (I) exhibited the most favorable antitoxoplasma activity without host toxicity. The binding mode of the synthesized N6-benzyladenosine analogs were characterized to illustrate the role of addnl. hydrophobic effect and van der Waals interaction within an active site of T. gondii adenosine kinase by induced fit mol. modeling.

IT 23707-32-6P 101565-87-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis, biol. evaluation and mol. modeling studies of N6-benzyladenosine analogs as potential anti-toxoplasma agents)

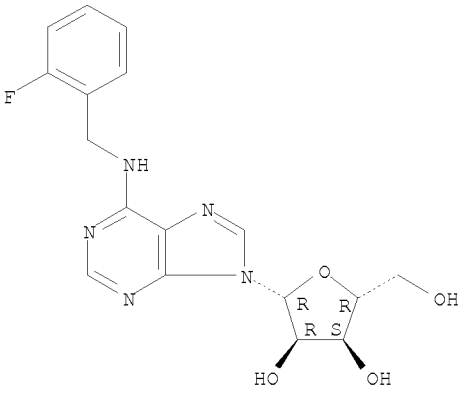
RN 23707-32-6 CAPLUS
CN Adenosine, N-[(2-chlorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 101565-87-1 CAPLUS
CN Adenosine, N-[(2-fluorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.

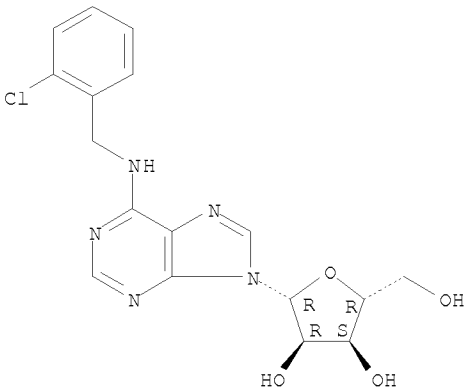


RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:245615 CAPLUS
DN 146:474750
TI Three-Dimensional Quantitative Structure-Activity Relationship of Nucleosides Acting at the A3 Adenosine Receptor: Analysis of Binding and Relative Efficacy
AU Kim, Soo-Kyung; Jacobson, Kenneth A.
CS Molecular Recognition Section Laboratory of Bioorganic Chemistry, National Institute of Diabetes and Digestive and Kidney Diseases (NIDDK), National Institutes of Health (NIH), Bethesda, MD, 20892, USA

SO Journal of Chemical Information and Modeling (2007), 47(3), 1225-1233
CODEN: JCISD8; ISSN: 1549-9596
PB American Chemical Society
DT Journal
LA English
AB The binding affinity and relative maximal efficacy of human A3 adenosine receptor (AR) agonists were each subjected to ligand-based three-dimensional quant. structure-activity relation anal. Comparative mol. field anal. (CoMFA) and comparative mol. similarity indexes anal. (CoMSIA) used as training sets a series of 91 structurally diverse adenosine analogs with modifications at the N6 and C2 positions of the adenine ring and at the 3', 4', and 5' positions of the ribose moiety. The CoMFA and CoMSIA models yielded significant cross-validated q2 values of 0.53 (r2 = 0.92) and 0.59 (r2 = 0.92), resp., and were further validated by an external test set (25 adenosine derivs.), resulting in the best predictive r2 values of 0.84 and 0.70 in each model. Both the CoMFA and the CoMSIA maps for steric or hydrophobic, electrostatic, and hydrogen-bonding interactions well reflected the nature of the putative binding site previously obtained by mol. docking. A conformationally restricted bulky group at the N6 or C2 position of the adenine ring and a hydrophilic and/or H-bonding group at the 5' position were predicted to increase A3AR binding affinity. A small hydrophobic group at N6 promotes receptor activation. A hydrophilic and hydrogen-bonding moiety at the 5' position appears to contribute to the receptor activation process, associated with the conformational change of transmembrane domains 5, 6, and 7. The 3D-CoMFA/CoMSIA model correlates well with previous receptor-docking results, current data of A3AR agonists, and the successful conversion of the A3AR agonist into antagonists by substitution (at N6) or conformational constraint (at 5'-N-methyluronamide).
IT 23707-32-6
RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)
(QSAR of nucleosides acting at A3 adenosine receptor)
RN 23707-32-6 CAPLUS
CN Adenosine, N-[(2-chlorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.

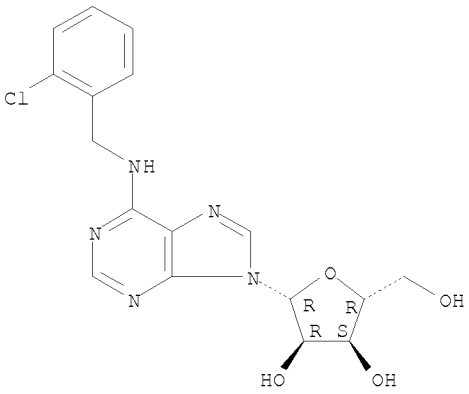


RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:44237 CAPLUS
DN 142:290603
TI A radial distribution function approach to predict A2B agonist effect of adenosine analogues
AU Gonzalez, Maykel Perez; Teran, Carmen; Fall, Yagamare; Teijeira, Marta; Besada, Pedro
CS Unit of Services, Department of Drug Design, Experimental Sugar Cane Station 'Villa Clara-Cienfuegos', Ranchuelo, Cuba
SO Bioorganic & Medicinal Chemistry (2005), 13(3), 601-608
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier Ltd.
DT Journal

LA English
AB The radial distribution function (RDF) approach has been applied to the study of the A2B agonist effect of a set of 89 adenosine analogs reported with this activity. A model able to describe more than 70% of the variance in the exptl. activity was developed with the use of the mentioned approach. In contrast, none of the eleven different approaches including the use of Constitutional, Topol., Mol. walk count, BCUT, Galvez topol. charge indexes, 2D autocorrelations, Randic mol. profiles, Geometrical, 3D Morse, WHIM and GETAWAY descriptors was able to explain more than 47% of the variance in the mentioned property with the same number of descriptors.
IT 23707-32-6
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(radial distribution function approach to predict A2B agonist effect of adenosine analogs)
RN 23707-32-6 CAPLUS
CN Adenosine, N-[(2-chlorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:566634 CAPLUS
DN 141:123865
TI Substitution derivatives of N6-benzyl-adenosine, methods of their preparation, their use for preparation of drugs, cosmetic preparations and growth regulators, pharmaceutical preparations, cosmetic preparations and growth regulators containing these compounds
IN Dolezal, Karel; Popa, Igor; Zatloukal, Marek; Lenobel, Rene; Hradecka, Dana; Vojtesek, Borivoj; Uldrijan, Stjepan; Mlejnek, Petr; Werbrouck, Stefaan; Strnad, Miroslav
PA Ustav Experimentalni Botaniky Akademie Ved Ceske Republiky, Czech Rep.; et al.
SO PCT Int. Appl., 114 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004058791	A2	20040715	WO 2003-CZ78	20031229
WO 2004058791	A3	20041028		

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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,

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ZA 2005006074 A 20060531 ZA 2005-6074 20050728
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WO 2003-CZ78 W 20031229
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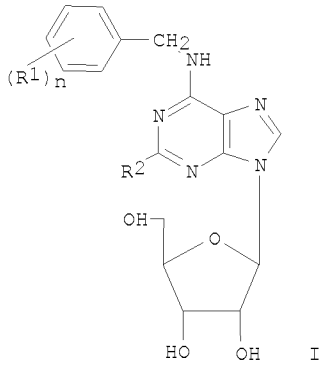


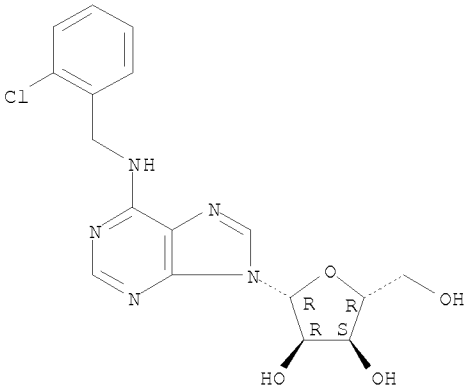
AB The invention concerns novel substitution derivs. of N6-benzyl-adenosine I, wherein n is 2-6; R1 is H, OH, halogen, alkoxy, amino, hydrazo, mercapto, methylmercapto, carboxyl, cyano, nitro, amido, sulfo, sulfamido, acylamino, acyloxy, alkylamino, dialkylamino, alkylmercapto, carbylalkoxy, cycloalkyl, carbamoyl alkyl; R2 is H, OH, halogen, alkoxy, amino, hydrazo, mercapto, methylmercapto, carboxyl, cyano, nitro, amido, sulfo, sulfamido, acylamino, acyloxy, alkylamino, dialkylamino, alkylmercapto, cabylalkoxy, cycloalkyl, carbamoyl, having anticancer, mitotic, immunosuppressive and anti-senescent properties for plant, animal and human cells. This invention also relates to the methods of preparation of these N6-benzyl-adenosine derivs. and their use as drugs, cosmetic prepns. and growth regulators comprising these derivs. as active compound and use of these derivs. for preparation of pharmaceutical compns., in biotechnol. processes, in cosmetics and in agriculture. Use of title compds. as mitotic or antimitotic compound, especially for treating cancer, psoriasis, rheumatoid arthritis, lupus, type I diabetes, multiple sclerosis, restenosis, polycystic kidney disease, graft rejection, graft vs. host disease and gout, parasitoses such as those caused by fungi or protists, or Alzheimer's disease, or as anti-neurogenerative drugs, or to suppress immunostimulation or for the treatment of proliferative skin diseases. Thus, 2-amino-6-(2-methoxybenzylamino)purine riboside was prepared as growth regulator, and antitumor agent.

IT 23707-32-6P 101565-87-1P 288087-35-4P
722505-02-4P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); COS (Cosmetic use); IMF (Industrial manufacture); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N6-benzyladenosine nucleosides as antitumor, mitotic, immunosuppressive prodrugs, cosmetic agents, and growth regulators)

RN 23707-32-6 CAPLUS

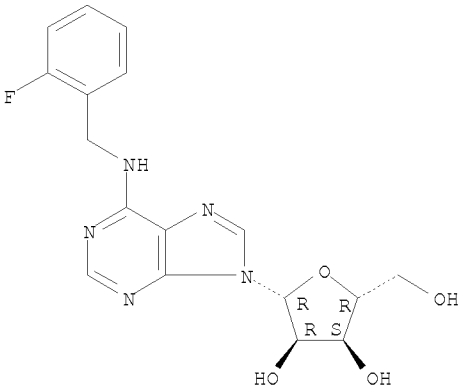
CN Adenosine, N-[(2-chlorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



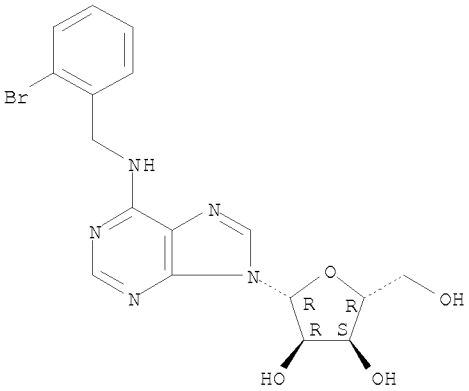
RN 101565-87-1 CAPLUS
CN Adenosine, N-[(2-fluorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



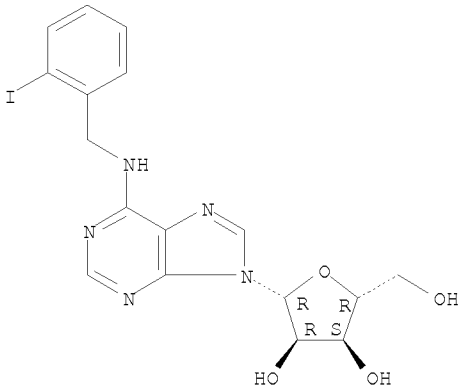
RN 288087-35-4 CAPLUS
CN Adenosine, N-[(2-bromophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 722505-02-4 CAPLUS
CN Adenosine, N-[(2-iodophenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

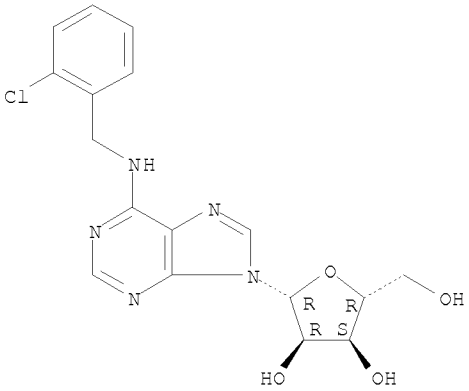


L8 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:368857 CAPLUS
DN 140:386000
TI Compounds, compositions and methods for modulating fat metabolism for treatment of metabolic disorders
IN Gaudriault, Georges; Kilinc, Ahmet; Bousquet, Olivier; Goupil-Lamy, Anne; Harosh, Itzik
PA Obetherapy Biotechnology, Fr.
SO PCT Int. Appl., 461 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004037159	A2	20040506	WO 2003-IL860	20031023
WO 2004037159	A3	20040715		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003274652	A1	20040513	AU 2003-274652	20031023
PRAI US 2002-420316P	P	20021023		
WO 2003-IL860	W	20031023		

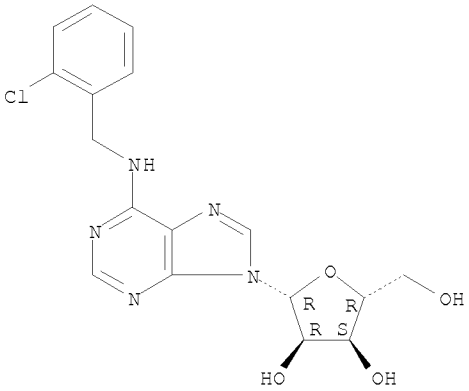
OS MARPAT 140:386000
AB Methods and compns. of identifying candidate compds., for modulating fat metabolism and/or inhibiting Apobec-1 activity are provided. The invention relates to compds. and pharmaceutical compns. which are useful for regulating fat metabolism and can be used for treatment of diseases and disorders selected from the group consisting of overweight, obesity, atherosclerosis, hypertension, non-insulin dependent diabetes mellitus, pancreatitis, hypercholesteremia, hypertriglyceridemia, hyperlipidemia.
IT 23707-32-6
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(compds., compns. and methods for modulating fat metabolism for treatment of metabolic disorders)
RN 23707-32-6 CAPLUS
CN Adenosine, N-[(2-chlorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



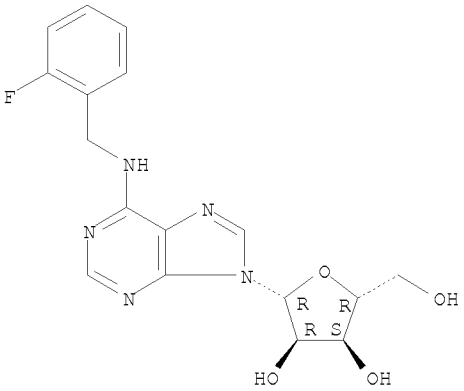
L8 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:364951 CAPLUS
DN 139:345305
TI N6-Substituted adenosine derivatives: selectivity, efficacy, and species differences at A3 adenosine receptors
AU Gao, Zhan-Guo; Blaustein, Joshua B.; Gross, Ariel S.; Melman, Neli; Jacobson, Kenneth A.
CS Laboratory of Bioorganic Chemistry, Molecular Recognition Section, National Institutes of Health, National Institute of Diabetes and Digestive and Kidney Diseases, Bethesda, MD, 20892, USA
SO Biochemical Pharmacology (2003), 65(10), 1675-1684
CODEN: BCPCA6; ISSN: 0006-2952
PB Elsevier Science Inc.
DT Journal
LA English
AB The activation of the human A3 adenosine receptor (AR) by a wide range of N6-substituted adenosine derivs. was studied in intact CHO cells stably expressing this receptor. Selectivity of binding at rat and human ARs was also determined Among N6-alkyl substitutions, small N6-alkyl groups were associated with selectivity for human A3ARs vs. rat A3ARs, and multiple points of branching were associated with decreased hA3AR efficacy. N6-Cycloalkyl-substituted adenosines were full (≤5 carbons) or partial (≥6 carbons) hA3AR agonists. N6-(endo-norbornyl)adenosine was the most selective for both rat and human A1ARs. Numerous N6-arylmethyl analogs, including substituted benzyl, tended to be more potent in binding to A1 and A3 vs. A2AARs (with variable degrees of partial to full A3AR agonisms). A chloro substituent decreased the efficacy depending on its position on the benzyl ring. The A3AR affinity and efficacy of N6-arylethyl adenosines depended highly on stereochem., steric bulk, and ring constraints. Stereoselectivity of binding was demonstrated for N6-(R-1-phenylethyl)adenosine vs. N6-(S-1-phenylethyl)adenosine, as well as for the N6-(1-phenyl-2-pentyl)adenosine, at the rat, but not human A3AR. Interestingly, DPMA, a potent agonist for the A2AAR (Ki=4 nM), was demonstrated to be a moderately potent antagonist for the human A3AR (Ki=106 nM). N6-[(1S,2R)-2-Phenyl-1-cyclopropyl]adenosine was 1100-fold more potent in binding to human (Ki=0.63 nM) than rat A3ARs. Dual acting A1/A3 agonists (N6-3-chlorobenzyl-, N6-(S-1-phenylethyl)-, and 2-chloro-N6-(R-phenylisopropyl)adenosine) might be useful for cardioprotection.
IT 23707-32-6, N6-(2-Chlorobenzyl)adenosine 101565-87-1, N6-(2-Fluorobenzyl)adenosine
RL: PAC (Pharmacological activity); BIOL (Biological study)
(N6-Substituted adenosine derivs. and selectivity, efficacy, and species differences at A3 adenosine receptors)
RN 23707-32-6 CAPLUS
CN Adenosine, N-[(2-chlorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 101565-87-1 CAPLUS
CN Adenosine, N-[(2-fluorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2000:720701 CAPLUS
DN 134:65798
TI Adenosine Analogues as Inhibitors of Trypanosoma brucei Phosphoglycerate Kinase: Elucidation of a Novel Binding Mode for a 2-Amino-N6-Substituted Adenosine
AU Bressi, Jerome C.; Choe, Jungwoo; Hough, Melinda T.; Buckner, Frederick S.; Van Voorhis, Wesley C.; Verlinde, Christophe L. M. J.; Hol, Wim G. J.; Gelb, Michael H.
CS Departments of Chemistry Biochemistry Medicine and Biological Structure, University of Washington, Seattle, WA, 98195, USA
SO Journal of Medicinal Chemistry (2000), 43(22), 4135-4150
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB As part of a project aimed at structure-based design of adenosine analogs as drugs against African trypanosomiasis, N6-, 2-amino-N6-, and N2-substituted adenosine analogs were synthesized and tested to establish structure-activity relationships for inhibiting Trypanosoma brucei glycosomal phosphoglycerate kinase (PGK), glyceraldehyde-3-phosphate dehydrogenase (GAPDH), and glycerol-3-phosphate dehydrogenase (GPDH). Evaluation of x-ray structures of parasite PGK, GAPDH, and GPDH complexed with their adenosyl-bearing substrates led the authors to generate a series of adenosine analogs which would target all three enzymes simultaneously. There was a modest preference by PGK for N6-substituted analogs bearing the 2-amino group. The best compound in this series,

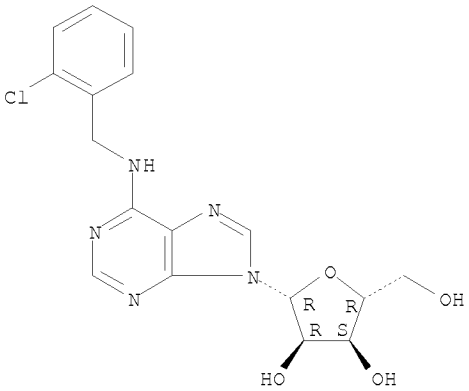
2-amino-N6-[2''-(p-hydroxyphenyl)ethyl]adenosine (I), displayed a 23-fold improvement over adenosine with an IC50 of 130 μM. 2-[[2''-(P-Hydroxyphenyl)ethyl]amino]adenosine was a weak inhibitor of T. brucei PGK with an IC50 of 500 μM. To explore the potential of an additive effect that having the N6 and N2 substitutions in one mol. might provide, the best ligands from the two series were incorporated into N6,N2-disubstituted adenosine analogs to yield N6-(2''-phenylethyl)-2-[(2''-phenylethyl)amino]adenosine as a 30 μM inhibitor of T. brucei PGK which is 100-fold more potent than the adenosine template. In contrast, these series gave no compds. that inhibited parasitic GAPDH or GPDH more than 10-20% when tested at 1.0 mM. A 3.0 Å x-ray structure of a T. brucei PGK/I complex revealed a binding mode in which the nucleoside analog was flipped and the ribosyl moiety adopted a syn conformation as compared with the previously determined binding mode of ADP. Mol. docking expts. using QXP and SAS program suites reproduced this "flipped and rotated" binding mode.

IT 23707-32-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(adenosine analogs as inhibitors of Trypanosoma brucei phosphoglycerate kinase and elucidation of a novel binding mode for a 2-amino-substituted adenosine)

RN 23707-32-6 CAPLUS

CN Adenosine, N-[(2-chlorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2000:369027 CAPLUS

DN 133:164255

TI A novel and facile reaction to N6-alkylated adenosine via benzotriazole as a synthetic auxiliary

AU Afify, Hanan M. N. M.; Pedersen, Erik B.; Zahran, Magdy A.

CS Chemistry Department, University of Southern Denmark, Odense University, Odense, DK-5230, Den.

SO Journal of Heterocyclic Chemistry (2000), 37(2), 339-341
CODEN: JHTCAD; ISSN: 0022-152X

PB HeteroCorporation

DT Journal

LA English

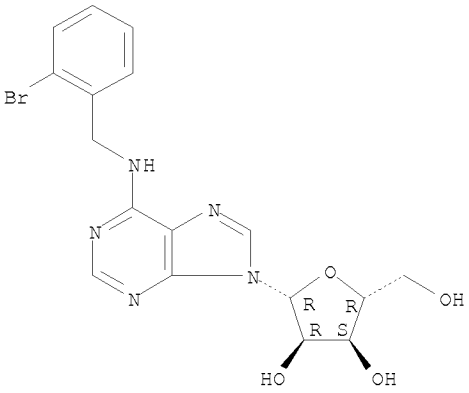
OS CASREACT 133:164255

AB The reaction of benzotriazole with aliphatic, aromatic or heteroarom. aldehyde and adenosine leads to a benzotriazole adduct which is reduced with sodium borohydride to the corresponding N6-alkylated adenosine derivs. This procedure is also utilized in a new route to N6-(3-iodobenzyl)adenosine-5'-N-methyluronamide (IB-MECA) which is considered an important adenosine agonist at A3 adenosine receptors.

IT 288087-35-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of N6-alkylated adenosines via benzotriazole intermediates)

RN 288087-35-4 CAPLUS
CN Adenosine, N-[(2-bromophenyl)methyl]- (CA INDEX NAME)

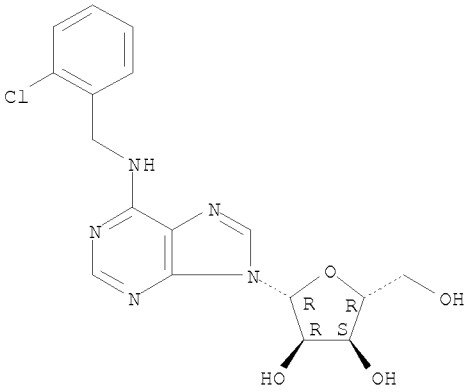
Absolute stereochemistry.



RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

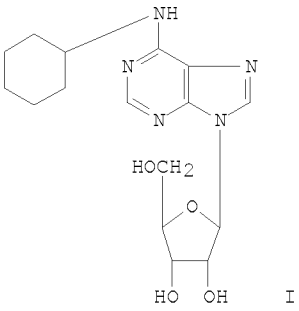
L8 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1998:329095 CAPLUS
DN 129:75990
TI A functional screening of adenosine analogs at the adenosine A2B receptor: a search for potent agonists
AU De Zwart, Maarten; Link, Regina; Von Frijtag Drabbe Kunzel, Jacobien K.; Cristalli, Gloria; Jacobson, Kenneth A.; Townsend-Nicholson, Andrea; Ijzerman, Ad P.
CS Division of Medicinal Chemistry, Leiden/Amsterdam Center for Drug Research, Leiden University, Leiden, 2300 RA, Neth.
SO Nucleosides & Nucleotides (1998), 17(6), 969-985
CODEN: NUNUD5; ISSN: 0732-8311
PB Marcel Dekker, Inc.
DT Journal
LA English
AB Various adenosine analogs were tested at the adenosine A2B receptor. Agonist potencies were determined by measuring the cAMP production in Chinese Hamster Ovary cells expressing human A2B receptors. 5'-N-Substituted carboxamidoadenosines were most potent. 5'-N-Ethylcarboxamidoadenosine (NECA) was most active with an EC50 value of 3.1 μM. Other ribose modified derivs. displayed low to negligible activity. Potency was reduced by substitution on the exocyclic amino function (N6) of the purine ring system. The most active N6-substituted derivative N6-methyl-NECA was 5 fold less potent than NECA. C8- and most C2-substituted analogs were virtually inactive. 1-Deaza-analogs had a reduced potency, 3- and 7-deazaanalogues were not active.
IT 23707-32-6
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(functional screening of adenosine analogs at adenosine A2B receptor: search for potent agonists)
RN 23707-32-6 CAPLUS
CN Adenosine, N-[(2-chlorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1988:105930 CAPLUS
DN 108:105930
TI Definition of subclasses of adenosine receptors associated with adenylate cyclase: interaction of adenosine analogs with inhibitory A1 receptors and stimulatory A2 receptors
AU Ukena, Dieter; Olsson, Ray A.; Daly, John W.
CS Natl. Inst. Arthritis, Diabetes, Dig. Kidney Dis., Natl. Inst. Health, Bethesda, MD, 20892, USA
SO Canadian Journal of Physiology and Pharmacology (1987), 65(3), 365-76
CODEN: CJPPA3; ISSN: 0008-4212
DT Journal
LA English
GI

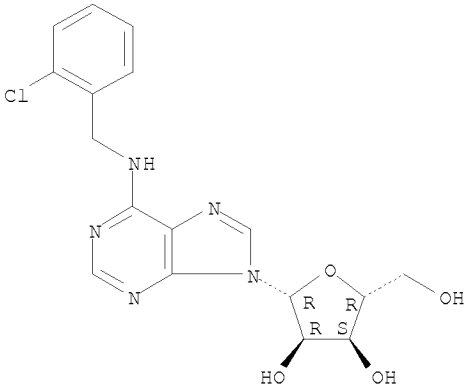


I

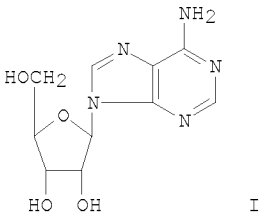
AB The structure-activity relationships of 63 adenosine analogs as agonists for the A1 adenosine receptors that mediate inhibition of adenylate cyclase activity in rat fat cells and for the A2 adenosine receptors that mediate stimulation of adenylate cyclase in rat pheochromocytoma PC12 cells and human platelets were determined The lack of correspondence between the structure-activity relationships of these analogs at the A1 and A2 receptors appear definitive in terms of estabishing the existence of A1 and A2 subclasses of adenosine receptors. However, significant differences in the agonist profiles at A2 receptors of platelet and PC12 indicate a certain degree of structural heterogeneity within the members of the A2 adenosine receptor subclass. Whether such differences are due to different species or different cell types is not known. A set of adenosine analogs, such as N6-cyclohexyl- (I), N6-R-, and N6-S-1-phenyl-2-propyladenosine, 5'-N-ethylcarboxamidoadenosine and its N6-cyclohexyl derivative, 2-chloroadenosine, and 2-phenylaminoadenosine, appear to represent a series of analogs useful for pharmacol. characterization of A1 and A2 classes of adenosine receptors.
IT 23707-32-6
RL: PRP (Properties)

(interaction of, with A1 and A2 adenosine receptors, of humans and laboratory animals)
RN 23707-32-6 CAPLUS
CN Adenosine, N-[(2-chlorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1986:603338 CAPLUS
DN 105:203338
OREF 105:32637a,32640a
TI Structure-activity relationships for N6-substituted adenosines at a brain A1-adenosine receptor with a comparison to an A2-adenosine receptor regulating coronary blood flow
AU Daly, John W.; Padgett, William; Thompson, Robert D.; Kusachi, Shozo; Bugni, William J.; Olsson, Ray A.
CS Lab. Bioorg. Chem., Natl. Inst. Arthritis, Diabetes, Dig. Kidney Dis., Bethesda, MD, 20205, USA
SO Biochemical Pharmacology (1986), 35(15), 2467-81
CODEN: BCPCA6; ISSN: 0006-2952
DT Journal
LA English
GI



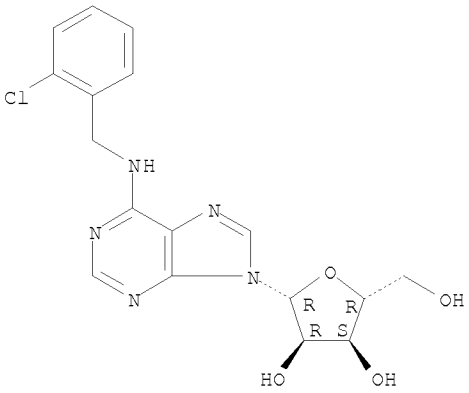
I

AB A series of 145 N6-substituted adenosine (I) analogs were screened as inhibitors of the binding of [3H]cyclohexyladenosine to a purinergic A1 receptor in rat brain membranes, and the results were compared to the potencies of these analogs in increasing coronary blood flow via activation of a purinergic A2 receptor. The A1 receptor shows greater stereoselectivity in the N6 region of the receptor towards asym. aralkyl substituents and shows greater bulk tolerance in the N6 region such that it retains affinity for certain N6-tertiary alkyladenosines and N6-cycloalkyladenosines that are inactive at the coronary A2 receptor. At the A1 receptor, the most potent analogs have either aliphatic N6-substituents with ≥4 methylene residues or have an N6-halophenyl substituent. At the A2 receptor, the most potent analogs have an N6-phenethyl or similar heteroarylethyl substituent. Certain sets or series of analogs appear useful for identifying the subtypes of purinergic receptors involved in physiol. functions.
IT 23707-32-6 101565-87-1

RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(purinergic receptor subtypes interaction with, structure in relation to)

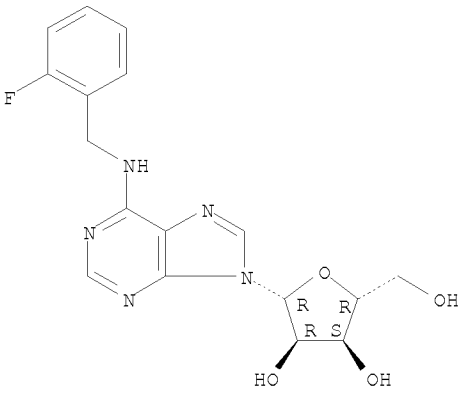
RN 23707-32-6 CAPLUS
CN Adenosine, N-[(2-chlorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.

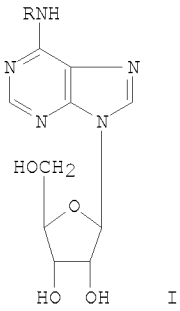


RN 101565-87-1 CAPLUS
CN Adenosine, N-[(2-fluorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1986:199592 CAPLUS
DN 104:199592
OREF 104:31391a,31394a
TI Dog coronary artery adenosine receptor. Structure of the N6-aryl subregion
AU Kusachi, Shozo; Thompson, Robert D.; Yamada, Noboyuki; Daly, Daniel T.; Olsson, R. A.
CS Coll. Med., Univ. South Florida, Tampa, FL, 33612, USA
SO Journal of Medicinal Chemistry (1986), 29(6), 989-96
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
GI



I

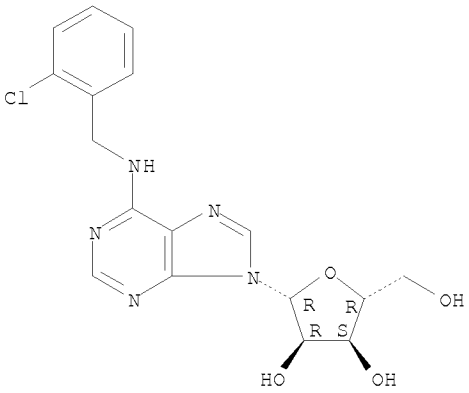
AB Ninety-two adenosine derivs. [I; R = 3-phenylpropyl, 4-phenylbutyl, 2,2-diphenylethyl, 2-(2-pyridyl)ethyl, halophenyl, 1-naphthyl, 3-indolyl, etc.), 47 of which were prepared by reaction of the appropriate amine with 6-chloropurine ribonucleoside [2004-06-0], were tested for adenosine receptor-binding activity in dog coronary arteries in vitro. The structure-activity relations of I drawn from these results are discussed with respect to the presence of an N6-aryl subregion in the coronary artery A2-adenosine receptor.

IT 23707-32-6
RL: BIOL (Biological study)
(adenosine receptor-binding activity of, in coronary artery, structure in relation to)

RN 23707-32-6 CAPLUS

CN Adenosine, N-[(2-chlorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.

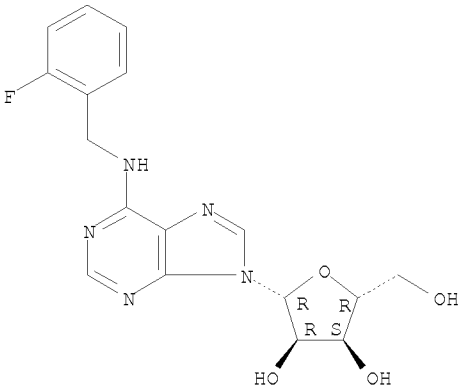


IT 101565-87-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and coronary artery adenosine receptor-binding activity of, structure in relation to)

RN 101565-87-1 CAPLUS

CN Adenosine, N-[(2-fluorophenyl)methyl]- (CA INDEX NAME)

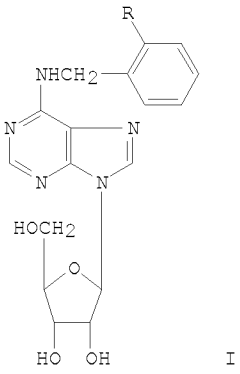
Absolute stereochemistry.



L8 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1985:488177 CAPLUS
DN 103:88177
OREF 103:14177a,14180a
TI Adenosine derivatives and their use as anticonvulsants
IN Irmscher, Klaus; Uhl, Juergen
PA Merck Patent G.m.b.H. , Fed. Rep. Ger.
SO U.S., 5 pp. Cont.-in-part of U.S. Ser. No. 303,295, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4514405	A	19850430	US 1984-573178	19840123
PRAI US 1981-303295	A2	19810917		

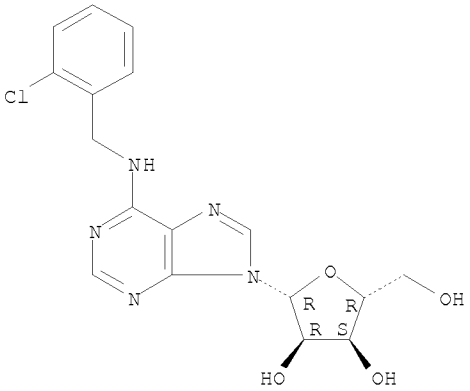
OS MARPAT 103:88177
GI



I

AB N6-Benzyladenosines I (R = H, Cl, F, Br, CF3), useful as anticonvulsants (no data), were prepared Thus, a mixture of 28.6 g 6-chloro-9-(β-D-ribofuranosyl)purine, 14.2 g o-ClC6H4CH2NH2, 400 mL DMF, 400 mL isopropanol, and 50 mL Et3N was allowed to stand 4 days at 20° to give I (R = Cl) (yield not given).
IT 23707-32-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23707-32-6 CAPLUS
CN Adenosine, N-[(2-chlorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.

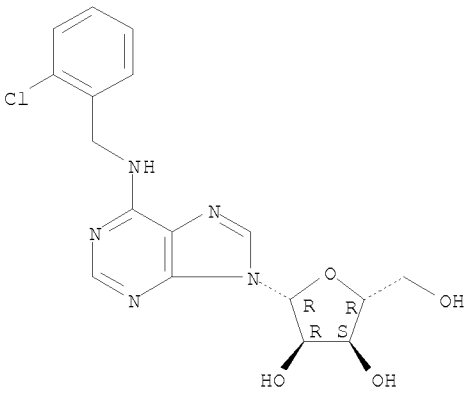


L8 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1969:115505 CAPLUS
DN 70:115505
OREF 70:21591a,21594a
TI N6-Aralkyl adenosine derivatives
IN Thiel, Max; Stach, Kurt; Jahn, Werner; Schaumann, Wolfgang; Dietmann, Karl
PA Boehringer, C. F., und Soehne G.m.b.H.
SO S. African, 15 pp.
CODEN: SFXXAB
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	ZA 6707414		19680502		
	DE 1670171			DE	
	FR 1550512			FR	
	GB 1145789			GB	
	US 3506643		19700414	US	19671018
PRAI	DE		19661209		
	DE		19670711		

OS MARPAT 70:115505
GI For diagram(s), see printed CA Issue.
AB The title compds. (1), where halogen, alkyl, alkoxy, F3C or alkylthio, or two substituents may be H or a methylenedioxy, are prepared from the corresponding D-ribosides and benzylamines, or from the corresponding N'-substituted adenosine derivs. Thus, 8.2 g. tri-O-acetyl-6-chloro-9-β-D-ribosyl-9-H-purine and 7.2 g. 2-ClC6H4CH2NH2 in 120 cc. iso-PrOH were refluxed 2 hrs., worked up and the residue dissolved in 100 cc. MeOH, 10 cc. N NaOH solution added and the mixture refluxed 1 hr. to yield 4 g. I (R = 2-Cl), m. 182-3°. The following I were similarly prepared (R and m.p. given): 3,4-Cl2, 182-3°; 4-MeO, 146-7°; 3,4(MeO)2, 135-6°; 3,4,5-(MeO)3, 118-19°; 2,6-Cl2, 207-9°; 4-Cl, 174-5°; 3-Cl, 168-9°; 2-MeO, 147-8°; 2-Me, 157-8°; 3,5-(MeO)2, 191-2°; 2-MeS, 127-8°; 2-F3C, 160-1°; and 3-F3C, 111-12°. To a suspension of 10 g. 2',3'-O-isopropylideneadeno-sine in 200 cc. MeCN, 10 g. p-BrC6H4Br was added and the mixture refluxed 24 hrs. with stirring. The precipitate which formed was filtered off, dissolved in 150 cc. MeOH and an equal volume 2N NaOH solution was added. The mixture was heated on a steam bath 20 min., extracted with CHCl3, evaporated, and the residue dissolved in 200 cc. HCO2N. Water was added until the mixture became cloudy. The mixture was left standing 1 day at ambient temperature, after which it was evaporated in vacuo, and the residue made weakly alkaline with an aqueous solution of concentrated NH3 to yield 5.8 g. I (R = 4-Br), m. 168-9°. I exhibit an effect on blood vessels and circulation.
IT 23707-32-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23707-32-6 CAPLUS
CN Adenosine, N-[(2-chlorophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.

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     (FILE 'HOME' ENTERED AT 21:57:00 ON 16 MAR 2008)

     FILE 'REGISTRY' ENTERED AT 21:57:24 ON 16 MAR 2008
                E 6-(2-FLUOROBENZYLAMINO)PURINE RIBOSIDE/CN
L1            1 S E2

     FILE 'CAPLUS' ENTERED AT 21:58:32 ON 16 MAR 2008
L2            7 S L1
L3            0 S L2 AND RIBOSIDE
L4            0 S L2 AND RIBOSE

     FILE 'REGISTRY' ENTERED AT 22:00:02 ON 16 MAR 2008
L5                STRUCTURE UPLOADED
L6            0 S L5
L7            4 S L5 FULL

     FILE 'CAPLUS' ENTERED AT 22:04:21 ON 16 MAR 2008
L8           15 S L7
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